

Burgers vector, Burgers circuit, and Dislocation Line Direction

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The 1st version of this white paper was written after the online discussion between Keonwook and Prof. Cai about Burgers vector on July 4, 2004, when it was just three days after Prof. Cai started his career as a professor at Stanford University. Let's start with Keonwook's question, which are quoted below from his email.

Q. Frank's rule says that Burgers vectors can be added just like vector summation. Weertman says the direction of dislocation should be same when Burgers vectors are added [1]. Here I just wonder how the direction of dislocation can be determined. Is there any conventional definition for that? I attached a figure(see Fig. 1) related with this question.

A. Yes, the Burgers vector of a dislocation depends on which direction we go along the dislocation line. In Weertman's book, Fig. 1(b), all line directions goes upward, thus $\mathbf{b}_3 = \mathbf{b}_1 + \mathbf{b}_2$. If on the other hand, we let all line directions go outward from the node, then we will have $\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 = 0$.

Without Burgers vector, we can not say how much and to what direction a part of a plane is relatively displaced from the other part which is distinguished by a line boundary, as we call the dislocation. It is important to know how we define size and direction of a Burgers vector and what we can say about the dislocation with a given Burgers vector. First of all, let's think about how the Burgers vector can be defined when a closed dislocation is given like Fig. 2(a). The procedure is explained in the following steps.

- Decide the line direction ξ at will, for example, counterclockwise as shown in Fig. 2(c).
- Make a Burgers circuit¹ around the loop according to the right hands rule.
- Cut the Burger circuit along the shifted surface. Mark start(S) and end(E) points.
- Make a vector, \mathbf{b} from the start point to the end point.

¹see the idea of Burgers circuit in J. P. Hirth and J. Lothe's *Theory of Dislocations* Krieger Publishing Company 1982

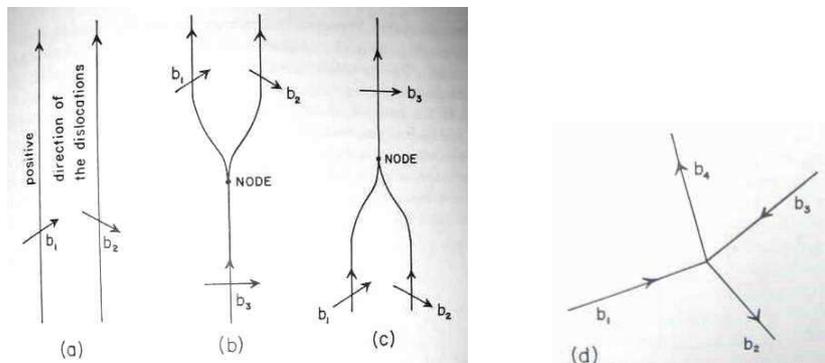


Figure 1: Examples of Burgers vector summation. In (b) and (c), $\mathbf{b}_1 + \mathbf{b}_2 = \mathbf{b}_3$ and in (d) $\mathbf{b}_1 + \mathbf{b}_3 = \mathbf{b}_2 + \mathbf{b}_4$. These figures are excerpted from the Weertman's book.

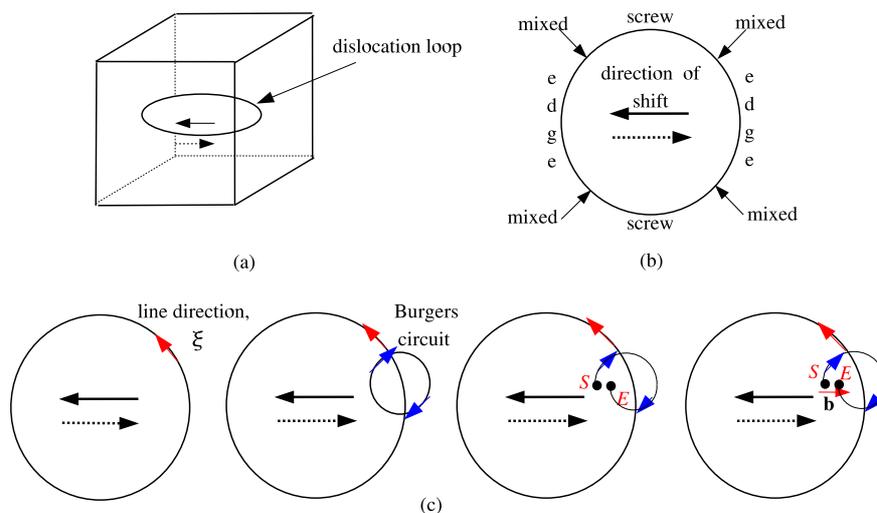


Figure 2: (a) A dislocation loop is created by shifting the upper half plane to the left with respect to the lower half within a loop area. (b) Edge, screw, and mixed dislocations all have the same Burgers vector. (c) The procedure to define a Burger vector \mathbf{b} is described step by step.

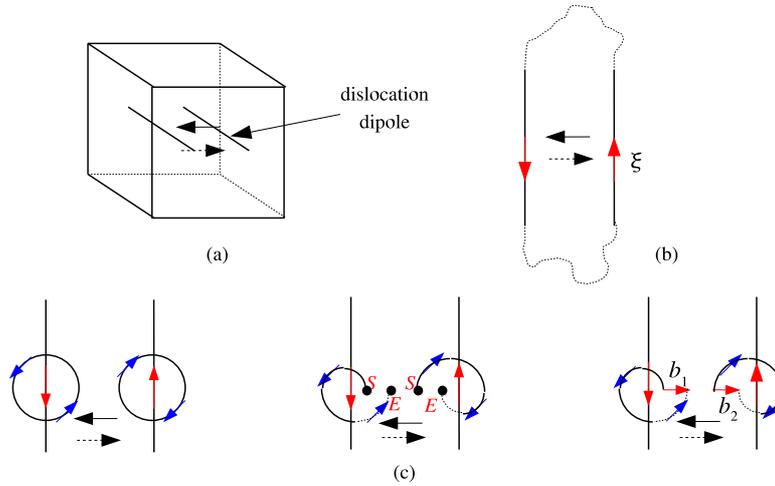


Figure 3: (a) A dislocation dipole is introduced into a perfect crystal. (b) The dipole can be thought as a part of a dislocation loop with its line direction chosen counterclockwise. In (c), it is shown that each dislocation has the same Burgers vector, $\mathbf{b} = \mathbf{b}_1 = \mathbf{b}_2$

Following this rule a.k.a. RH/SF (right hand and start-to-final) convention, we can easily define size and direction of a Burgers vector, although the convention could be different from book to book on dislocation theory. Note that, if the clockwise line direction, ξ is chosen, the direction of Burgers vector would be the opposite. Thus, keep it in mind that when you say the direction of Burger vector, you have to specify what direction you chose as a line direction.

Let's see another example of a dislocation dipole, a pair of straight dislocations whose Burgers vectors have the same magnitude but the opposite sign. This dislocation pair can be thought as a part of a dislocation loop. From Fig. 3, it is shown that each dislocation has the same burger vector $\mathbf{b} = \mathbf{b}_1 = \mathbf{b}_2$ from the RH/SF convention when the line direction of one dislocation is opposite to that of the other dislocation. Thus, we can see that, if we choose the line direction of both dislocations to be headed for the same direction, the sign of two Burgers vectors become opposite to each other which is in accordance with the definition of a dislocation dipole

At this point, let's think about what would happen if two dislocations meet. According to the Weertman's convention, the line direction of two dislocations should be same when their Burgers vectors are added. So, both line directions are taken upward as shown in Fig. 4(a). In this case, the line direction of the left dislocation is reversed, which makes the Burger vector \mathbf{b}_1 has negative sign in front of it. In Fig. 4(b), dislocations meet partially where the total Burgers vector becomes zero due to the vector addition of the same length but the opposite sign. This is equivalent to the fact that the Burgers circuit

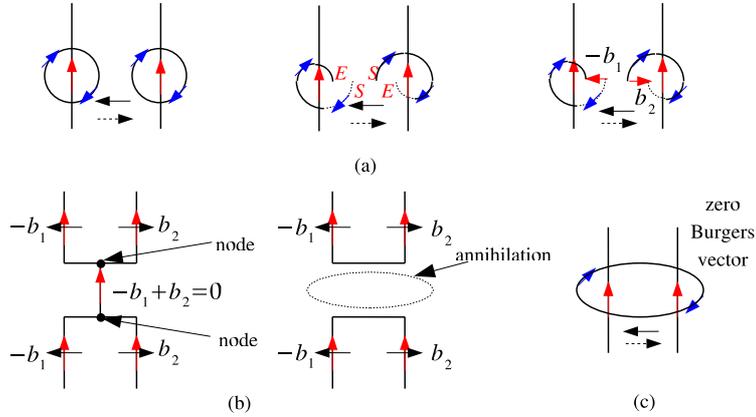


Figure 4: (a) The line directions are both taken upward direction. The Burgers vector is $-\mathbf{b}_1 = \mathbf{b}_2 = \mathbf{b}$. (b) When dislocations with the Burgers vector of the opposite sign meet each other, annihilation can happen. (c) The Burgers vector of the Burgers circuit surrounding a dislocation dipole is zero.

surrounding a dislocation dipole has zero Burgers vector.² (See Fig. 4(c).)

Up to now, we have talked about how the Burgers vector can be determined for a given dislocation once we know the direction of plane shift. Actually, the reverse approach can also be done similarly. For example, let's think about how we find the shift direction when the Burgers vector and the line direction are given like Fig. 5(a). The answer is given in Fig. 5(b). Once the Burgers vector is given with the line direction, the magnitude of the shift and its relative direction can be inferred. The choice of line direction is arbitrary, but you have to keep the direction in your problem once you decide it.

Now let's move onto the topic about dislocation network. (See Fig. 6.) We call a junction point as a node when two or more dislocations meet at that point. In this network, how do we perform Burgers vector summation around a node? The convention is to take the line direction along the radial direction from the node. Then Frank's rule of the conservation of Burgers vector says that the net Burgers vector \mathbf{b}_{net} must be zero. The vector sum of Burgers vectors is

$$\mathbf{b}_{net} = \mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 + \mathbf{b}_4 + \mathbf{b}_5 = 0$$

We can determine one unknown Burgers vector when all the other Burgers vectors are given.

²This explains the reason why the minimum number of dislocations introduced in a computation cell should be two for the periodic boundary condition. See Vasily B. Bulatov and Wei Cai, *Computer Simulations of Dislocations* Oxford University Press 2006 Ch.5

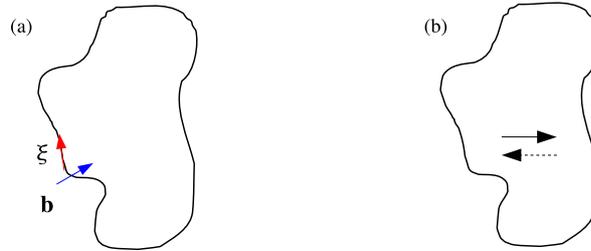


Figure 5: (a) The Burgers vector \mathbf{b} and the line direction, ξ of a dislocation loop. (b) The actual shift direction can be inferred such that the upper plane moves to the right and the bottom plane to the left.

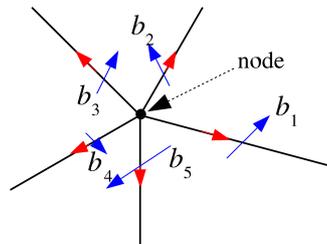


Figure 6: Dislocation network. The line direction (denoted as red arrows) is conventionally chosen to be outgoing direction from the node.

References

- [1] Johannes Weertman and Julia R. Weertman, *Elementary Dislocation Theory*, Oxford University Press 1992